XAFS Measurements of Li-NH₃ Solutions by Using X-ray Raman Scattering

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Introduction: Lithium (Li) metal can be dissolved in ammonia (NH₃) without chemical reaction. At about 5 mole percent metal (MPM), metal-non-metal transition occurs in the solutions, and above 8MPM the systems are metallic. The structure of the Li-NH₃, in particular, the local structure around NH₃, is not completely understood yet. For structural investigation of solutions, the XAFS spectroscopy is an appropriate technique, but direct XAFS measurements of N atoms (N-XAFS) in liquids are virtually impossible. However, by using X-ray Raman scattering (XRS), the N-XAFS in the Li-NH₃ is potentially measurable, if incident photon-flux is high enough.

Methods and Materials: The XRS spectrometer, consisting of a Johann-type Ge(440) having a 550mm radius of curvature and a 100mm-long position sensitive detector, was set at X14A. XRS spectra for liquid NH_3 (insulator), the 6MPM solution (semi-conductor), and the 14MPM solution (liquid metal) have been measured with $5\sim8$ eV resolution at momentum transfer, 5.6\AA^{-1} , under 218K.

Results: Fig. 1 shows the XRS spectra around the N-edge. In the three samples measured, a 'white line' is clearly found at 400eV. No marked peak shift among these spectra suggests that the chemical state of NH $_3$ molecules in the Li-NH $_3$ is similar to that in pure NH $_3$ liquid, in spite of the differences of macroscopic properties. Unfortunately, the S/N ratio of the XRS spectra is still insufficient to discuss the details of the N-XAFS features. The edge-jump is about 2000 counts for 2 days accumulation under ~10 12 photons/sec irradiation of X14A. We may need the flux, ~10 14 photons/sec, which might be achievable in the 3 rd generation synchrotron sources.

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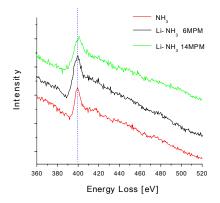


Figure 1. X-ray Raman scattering spectra of Li-NH₃ solutions.